SEMESTER - IV

ADVANCED NATURAL PRODUCTS

1. Course Description

Programme: **M.Sc.**
Course Code: P24/CHE/DSE/401
Course Type: **DSE –5**
No. of credits: 3

Max. Hours: 45
Hours per week: 3
Max. Marks: 100

2. Course Objectives

- To determine the biosynthetic mechanism through Acetate –malonate and, Shikimmic acid pathway and total synthesis for secondary metabolites.
- To elucidate the structure and discuss the stereochemistry of Natural products like Rotenone, Cholesterol, Reserpine and Abietic acid.
- To study the Structure of Natural products through Spectroscopic technique.

3. Course Outcomes

CO1: Assess the biosynthetic mechanism through Acetate –malonate and, Shikimmic acid pathway for secondary metabolites and to outline the total stereoselective synthesis including Corey's Synthesis of Prostaglandins and Paeoriflorin, sharpless synthesis of L-Hexoses, Takasago synthesis of Menthol, Hoffmann-LaRoche synthesis of Biotin **(UNDERSTANDING).**

CO2: Determine structure and stereochemistry of Reserpine, Abietic acid, Cholesterol and Rotenone **(APPLY)**

CO3: Determine the structure of natural products through Spectroscopic techniques **(APPLY).**

4. Course Content

MODULE I: BIOSYNTHESIS AND TOTAL STEREOSELECTIVE SYNTHESIS OF NATURAL PRODUCTS (15Hrs)

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation

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and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labelled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. Corey's synthesis of prostaglandins (E2, F2α) and paeoriflorin, Sharpless synthesis of L-hexoses, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

MODULE II: STRUCTURE DETERMINATION OF NATURAL PRODUCTS-I (15Hrs)

Determination of structure and stereochemistry of Reserpine, Abietic acid, Rotenone and Cholesterol.

MODULE III: STRUCTURE DETERMINATION OF NATURAL PRODUCTS-II

Spectroscopic techniques IR, UV, ^{1}Hnmr, ^{13}Cnmr, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

Study of the following solved problems: Mass, IR,^{1}H,^{13}C NMR, HOMOCOSY,HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of menthol, APT of apparicine, NOESY of buxaquamarine, 2D-INADEQUATE of α-picoline and β-methyl tetrahydranfuran

5. References

1. Biosynthesis by Geismann
2. Classics in total synthesis K C Nicolaou and E J Sorenson
3. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
4. An introduction to the chemistry of terpenoids and steroids, by William templeton
5. Total synthesis of Natural Products by Apsimon Vol 1-5
6. Systematic identification of flavonoid compounds by Mabry &Markham
7. Steroids by Fieser arid Fieser
8. Alkaloids by Manske
9. Alkaloids by Bentley
10. Alkaloids by Pelletier
11. Principles of organic synthesis 3rdEd.R O C Norman and J M Coxen
12. One and two dimensional nmr spectroscopy by Atta Ur Rahman
13. Spectrometric identification of organic compounds by Silverstein and Webster

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6. Syllabus Focus

a) Relevance to Local , Regional , National and Global Development Needs

Local /Regional/National /Global Development Needs	Relevance
National	Natural product biosynthesis is used in a variety of industries, including cosmetics, nutrition and food technology, and medicine.
Global	Industrially viable production of one stereochemical isomer through total stereoselective synthesis of natural products.
Local	Elucidate new mechanisms of action, providing exciting new avenues in drug discovery.
Regional	Spectral interpretation of Natural products to deduce the structure

b) Components on Skill Development/Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No. 1	Comparing the biosynthetic mechanisms with laboratory synthesis
ED	Module No.2	Encourage students to reflect on the skills and knowledge required to pursue entrepreneurship in the field of natural product structural determination.
EMP	Module No. 3	Encourage discussions on the challenges faced, uncertainties in the predictions, and alternative interpretations of the spectral data in the pharmaceutical industry.

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7. Pedagogy

S. No.	Student Centric Methods Adopted	Type / Description of Activity
1.	Seminars/Assignment	Participative Learning
2.	Science Experiments	Experiential Learning
3.	Case studies	Problem solving

8. Course Assessment Plan

a) Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA - 40%	End Semester Examination-60%
CO1	CIA1-Written Exam	Written Exam
CO2	Skill Test-I – Assignment	
CO3	Skill Test-II - Presentation	

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MODEL QUESTION PAPER

THEORY

Course Code: P24/CHE/DSE/403 **Max Marks:60**

Credits: 3 **Max Hours:2½hrs**

SECTION A - INTERNAL CHOICE
3Q X 12 M = 36 M

Question Number	Module	Question	CO	BTL
1	Module 1	(a) Describe the shikimic acid pathway for the biosynthesis of aromatic compounds (b) Write the Corey's synthesis of Prostaglandins	CO 1	Level II Level I
2	Module 1	(a) Deduce the biosynthetic pathway of flavonoids (b) Discuss the Sharpless synthesis of L-Hexoses.	CO 1	Level II Level II
3	Module 2	(a) Discuss the structure determination of Rotenone (b) Explain the stereochemistry of Cholesterol	CO 2	Level II Level II
4	Module 2	(a)Describe how the structure of Reserpine was established (b) Write stereochemistry of Abietic Acid	CO 2	Level II Level I
5	Module 3	(a)Explain the structural elucidation of Quinolines by IR, UV, ^{1}HNMR, ^{13}CNMR spectral Analysis (b)Discuss NOESY of Geraniol	CO 3	Level II Level II
6	Module 3	(a)Explain the spectral analysis of monoterpenes (b)Briefly explain 2D-INADEQUATE spectrum of α-Picoline and β-MethylTetrahydranfuran	CO 3	Level II Level II

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SECTION B - ANSWER ANY 4 OUT OF 6 **4 Q X 6 M = 24 M**
(To compulsorily have ONE questions from each module)

7	Module 1	What are the differences between a laboratory synthesis and biosynthesis?	CO 1	Level I
8	Module 1	Explain the Takasago synthesis of Menthol.	CO 1	Level II
9	Module 2	How do you determine the position of double bond in Cholesterol?	CO 2	Level I
10	Module 2	Discuss the stereochemistry of Reserpine	CO 2	Level II
11	Module 3	Explain the UV spectral analysis of Flavanoid taking suitable examples.	CO 3	Level II
12	Module 3	Briefly give the Mass spectral and ^{1}H NMR analysis of Umbelliferone	CO 3	Level I

b) Model Question Paper- End Semester Exam

ADVANCED NATURAL PRODUCTS
MODEL QUESTION PAPER
THEORY

Course Code: P24/CHE/DSE/401 **Max Marks:60**
Credits: 3 **Max Hours:2½hrs**

SECTION-A

I. Answer the following questions **3X12=36 Marks**

1. a) Describe the shikimic acid pathway for the biosynthesis of aromatic compounds.(CO1) (Level-1)
b) Write the Corey's synthesis of Prostaglandins. (CO1) (Level-1)

OR

2. (a) Deduce the biosynthetic pathway of flavonoids. (CO1) (Level-5)
(b) Discuss the Sharpless synthesis of L-Hexoses. (CO1) (Level-1)

3. (a) Discuss the structure determination of Rotenone (CO2) (Level-1).
(b) Explain the stereochemistry of Cholesterol (CO2) (Level-2).

OR

4. (c) Describe how the structure of Reserpine was established? (CO2) (Level-2).
(d)Write stereochemistry of Abietic Acid (CO2) (Level-1).

5. (a) Explain the structural elucidation of Quinolines by IR, UV, ^{1}HNMR, ^{13}CNMR spectral Analysis (CO3) (Level-2).
(b) Discuss NOESY of Geraniol. (CO3) (Level-1).

OR

6. (c) Explain the spectral analysis of monoterpenes (CO3) (Level-2).
(d) Briefly explain 2D-INADEQUATE spectrum of α-Picoline and β-MethylTetrahydranfuran (CO3) (Level-2).

SECTION-B

II Answer any <u>four</u> questions **4 X 6 = 24**

7.What are the differences between a laboratory synthesis and biosynthesis? (CO1) (Level-1)
8. Explain the Takasago synthesis of Menthol. (CO1) (Level-2)
9. How do you determine the position of double bond in Cholesterol? (CO2) (Level-1)
10. Discuss the stereochemistry of Reserpine.(CO2) (Level-2)
11. Explain the UV spectral analysis of Flavanoid taking suitable examples. (CO3) (Level-2)
12. Briefly give the Mass spectral and ^{1}H NMR analysis of Umbelliferone.(CO3) (Level-1)

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SEMESTER-IV **PRACTICALS**

CHEMISTRY LAB: DSE- 401
Program: M.Sc.
Course: DSE-V
Semester: IV

LAB:- Chemistry Software Programmes
Subject Code P24/CHE/DSE/401/P
No. of Hrs. allotted: 4 Hrs / week
No. of Credits :2

COURSE OUTCOMES:

CO1: To analyze IR and NMR spectra of organic compounds using ACD/IdNMR processor. Drawing graphs using EXCEL, Molecular docking by iGEM Docking software

Lab course 4 **Chemistry Software Programmes** **4 hrs/week**

Chem Draw
Analysis of IR and NMR using ACD/Id NMR processor.
EXCEL: Drawing graphs
Sequence retrieving from NCB, PDB-Structures and active site identification interactions in PDB
Molecular docking (iGEMDOCK).
Sequence Retrieving from NCBI
PDB - Structures, Active site Identification and Interactions in PDB

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MODEL PRACTICAL QUESTION PAPER

SEMESTER 1V

Paper IV : Practice of Chemistry Software Programmes

TIME: 3hrs **CourseCode: P24/CHE/DSE/401/P**
Max. Marks: 50

Q1. To analyze IR and NMR spectra of organic compounds using ACD/IdNMR Processor. **(CO1)** **10 M**

Q2. Write about Molecular docking by iGEM Docking software and interpret the results. **(CO1)** **25 M**

Q3. Record + Attendance **5 M**

Q4. Viva voce **10 M**

Prepared by Course Teacher [Name & Signature]	Checked &verified by HOD [Name & Signature]	Approved by the Principal
K. Susmitha Dr.K.Susmitha Dr.Sabiha Fatima	D. Sumalatha Dr. D. Sumalatha	Dr. Uma Joseph

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SEMESTER-IV

DRUG DESIGNANDDRUGDISCOVERY

1. Course Description

Programme: M.Sc. Organic Chemistry
Course Code: P24/CHE/DSC/401
Course Type: DSC-11
No. of credits: 3

Max. Hours: 45
Hours per week: 3
Max. Marks: 100

2. Course Objectives

b. To identify compounds that target specific disease processes, have high potency, low toxicity, and good pharmacokinetic properties.

c. To develop drugs that can be used to improve patient outcomes and quality of life.

3.Course Outcomes

CO1: Explain the various stages involved in drug discovery. **(UNDERSTANDING)**

CO2: Apply the various Lead modification strategies and also Structure Activity Relationship studies in drug development process. **(APPLICATION)**

CO3: Determine how the different physicochemical characteristics of drug molecules relate to biological activity .When developing new medicinal compounds, utilize a variety of QSAR study tools. **(APPLICATION)**

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4.Course Content

MODULE I: PRINCIPLES OF DRUG DESIGN AND DRUG DISCOVERY (15Hrs)

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists , antagonists and enzyme inhibitors . Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

MODULE II: LEAD MODIFICATION AND SAR STUDIES (15 Hrs)

Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs.

MODULE III: QSAR STUDIES AND COMPUTER AIDED DRUG DESIGN (15 Hrs)

QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).

Computer aided drug design: Introduction, active site, allosteric binding site, use of grids in docking,rigid docking, flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

5. References

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11.Organic and Pharmaceutical chemistry by Delgrado
12. Organic Pharmaceutical chemistry by Harikishan singh
13. Medicinal Chemistry by Ashtoshkar
14. Medicinal Chemistry by Chatwal
15. Organic Drug synthesis by Ledneicer Vol 1-6
16. Strategies for organic drug synthesis and design by Daniel Ledneicer.
17. Top Drugs: Top synthetic routes by John Saunders
I8.Chirotechnoiogy by Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol.1.
20. Medicinal Chemistry by G. Patricks.
21.Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tomm Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342-6363.

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1. Syllabus Focus

a) Relevance to Local, Regional, National and Global Development Needs

Local /Regional/National /Global Development needs	Relevance
REGIONAL	Drug design and drug discovery can foster collaborations between countries to tackle common health challenges and contribute to regional health initiatives.
NATIONAL	Drug design and discovery can advance the pharmaceutical sector and generate employment.
GLOBAL	Drug designing by SAR and QSAR studies plays a crucial role in developing new medications to address global health challenges like infectious diseases, cancer, and other chronic conditions.

b) Components on Skill Development/Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No. 1	Solving theoretical problems and interpreting results.
ED	Module No.2	Research collaborations
EMP	Module No. 3	Encourage critical thinking on research methodologies and applications from publications in journals

2. Pedagogy

S. No	Student Centric Methods Adopted	Type/ Description of Activity
1.	Problem Solving	Case studies
2.	Participative Learning	Presentation
3.	Experiential Learning	Field Trips

3. Course Assessment Plan

a) Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA- 40%	EndSemesterExamination-60%
CO1	CIA-1 - Written Exam	Written Exam
CO2	CIA-2 – Presentation	
CO3	CIA-2 – Assignment	

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b) Model Question Paper-End Semester Exam

DRUG DESIGN AND DRUG DISCOVERY
MODEL QUESTION PAPER
THEORY

TIME: 21/2hrs
Max. Marks: 60

Course Code: P24/CHE/DSC/401

Question Number	Module	Question	CO	BTL
1	Module 1	(a) Explain the various stages involved in drug discovery process. (b) Discuss the development of Captopril from Lead molecule.	CO 1	Level -II Level -I
2	Module 1	(c) Discuss the lead modification by structure pruning technique with morphine as an example. (d) Explain the occupancy theory in detail.	CO 1	Level -II Level -II
3	Module 2	(a)Explain the SAR in Sulfa drugs. (b) Discuss the development and discovery of Oxaminquine.	CO 2	Level –II Level -II
4	Module 2	(c) Discuss the concept of bio isosterism in the development of a lead. (d) Explain the concept of structure extension, ring expansion and ring variation in the development of drugs.	CO 2	Level -II Level -II
5	Module 3	(a)Explain the linear and non linear relationship between log P and biological activity. (b) How is Craig's Plot important in the Lead Development Programme.	CO 3	Level -II Level -II
6	Module 3	(c) Explain Topliss method of Lead Modification. (d) What is CADD? Explain the difference between Structure based and ligand based drug design.	CO 3	Level -II Level -II

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SECTION B - ANSWER ANY 4 OUT OF 6 (To compulsorily have **TWO** questions from **each** module)			**4Q X 6M = 24 M**	
7	**Module 1**	What are Folkore drugs?	**CO 1**	**Level -II**
8	**Module 1**	Discuss about the Pharmacokinetics of the drug.	**CO 1**	**Level -I**
9	**Module 2**	Discuss the Binding role of Hydroxyl and aromatic ring.	**CO 2**	**Level –I**
10	**Module 2**	Explain in brief Chain Homologation	**CO 2**	**Level -II**
11	**Module 3**	What is Hansch Analysis? Explain its use in Drug Discovery.	**CO 3**	**Level -II**
12	**Module 3**	Write a short note on Docking Studies of Drug Molecules.	**CO 3**	**Level -I**

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b) Model Question Paper-End Semester Exam

DRUG DESIGN AND DRUG DISCOVERY
MODEL QUESTION PAPER
THEORY

TIME: 21/2hrs **Course Code:**
P24/CHE/DSC/401
Max. Marks: 60

SECTION –A (Essay Questions)

I Answer the following questions **3X12=36**
Marks

1. (a) Explain the various stages involved in drug discovery process. **(CO1) (Level- II)**
   (b) Discuss the development of Captopril from Lead molecule. **(CO1) (Level - I)**

OR

2. (c) Discuss the lead modification by structure pruning technique with morphine as an example. **(CO1) (Level -I)**
   (d) Explain the occupancy theory in detail. **(CO1) (Level -II)**

3. (a)Explain the SAR in Sulfa drugs. **(CO2) (Level- II)**
   (b) Discuss the development and discovery of Oxaminquine**(CO2) (Level- II)**

OR

4. (c) Discuss the concept of bio isosterism in the development of a lead. **(CO2) (Level -II)**
   (d) Explain the concept of structure extension, ring expansion and ring variation in the development of drugs. **(CO2) (Level- II)**

5. (a)Explain the linear and non linear relationship between log P and biological activity. **(CO3) (Level -II)**
   (b) How is Craig's Plot important in the Lead Development Programme. **(CO3) (Level -II)**

OR

6. (c) Explain Topliss method of Lead Modification.**(CO3) (Level -II)**

(d) What is CADD? Explain the difference between Structure based and ligand based drug design. **(CO3) (Level -II)**

SECTION –B (Short Answer Questions)

II Anwer any four of the following questions **4 X 6 = 24 M**

7. What are Folkore drugs? **(CO1) (Level -II)**
8. Discuss about the Pharmacokinetics of the drug. **(CO1) (Level-1)**
9. Discuss the Binding role of Hydroxyl and aromatic ring. **(CO2) (Level-1)**
10. Explain in brief Chain Homologation**(CO2) (Level -II)**
11. What is Hansch Analysis? Explain its use in Drug Discovery. **(CO3) (Level - II)**
12. Write a short note on Docking Studies of Drug Molecules **(CO3) (Level-1)**

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c) Question Paper Blue print

Modules	Hours Allotted in the Syllabus	COs Addressed	Section A (No. of Questions)	Total Marks	Section B (No. of Questions)	Total Marks
1	15	1	2	12	2	4×6 = 24
2	15	2	2	12	2	
3	15	3	2	12	2	

4. CO-PO Mapping

CO	PO	Cognitive Level	Class room sessions (hrs)
1	2	Remembering	15
2	2	Evaluation	15
3	5	Apply	15

SPECTROSCOPIC IDENTIFICATION OF ORGANIC COMPOUNDS PRACTICAL

Programme M.Sc.
Course code: P24/CHE/DSC/401/P
Course : DSC XI
No. of Credits-2

Max. Marks: 50
No. of Hrs/Week: 4Hrs

COURSE OUTCOME

CO1: Interpretation of IR, UV, 1H -NMR, 13C NMR, and mass spectral data to identify the structure of unknown organic molecules.

Spectroscopic identification of Organic Compounds

Identification of unknown organic compounds by interpretation of IR, UV, 1H - NMR, 13C NMR, and mass spectral data (two examples with 2D-NMR).
A minimum of 30 representative examples should be studied.

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References :

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt
College publishers).
2.Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed.John Wiley and Sons.
3. Spectroscopic methods in organic chemistry - D. H. Williams and I Flemming McGraw Hill
4. Absorption spectroscopy of organic molecules – V. M. Parikh
5. Nuclear Magnetic Resonance – Basic Principles- Atta-Ur-Rehman, Springer-Verlag (1986).
6. One- and Two-dimensional NMR Spectroscopy – Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998)
8. Organic structural Spectroscopy- Joseph B.Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).
9. Organic structures from spectra –Field L.D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sons Ltd.

SPECTROSCOPIC IDENTIFICATION OF ORGANIC COMPOUNDS
MODEL PAPER
PRACTICAL

Course Code: P24/CHE/DSC/401/P Max
Time:3hrs
Credits: 2 Max marks
:50 marks

1) Interpret the given spectral data (IR, UV, 1H -NMR, 2D-NMR, 13C NMR, Mass) of two compounds and deduce the structures by following a systematic procedure? **(CO1)** **2**
x17½ =35M

2) Record +Attendance 5M

3) Viva 10M

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SEMESTER-IV

1.Course Description

Programme: M.Sc. Organic Chemistry
Course Code: P24/CHE/DSC/402
CourseType: DSC-XI1
No. of credits: 3

Max.Hours: 45
Hoursper week: 3
Max. Marks: 100

2.Course Objectives

- Drugs acting on metabolic process, cell wall and specific enzymes Sulphonamides were used to successfully treat many infections which later yielded to penicillin and so their role deserves wider acknowledgement
- Intercalation is the insertion of molecules between the planar bases of deoxyribonucleic acid (DNA). This process is used as a method for analyzing DNA and it is also the basis of certain kinds of poisoning
- Drugs interact with receptors by bonding at specific binding sites. Most receptors are made up of proteins, and the drugs can therefore interact with the amino acids to change the conformation of the receptor proteins.

3.Course Outcomes

CO1: Explain the basic concepts of mechanism of drug action. Outline the discovery and mechanism of action of the drugs acting on metabolic processes or antifolates. Describe the structure of bacterial cell wall and discuss the synthesis and mechanism of action of penicillins and cephalosporins on the bacterial cell wall (UNDERSTANDING)

CO2: Discuss the classification and mechanism of action of drugs acting on genetic material
(APPLICATION)

CO3: Give an overview of the nervous system, describe the structure of neuron and nerve
transmission. Discuss about the classification, synthesis and mode of action of drugs acting on
the various receptors (APPLICATION)

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UCS, Osmania University
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4 .Course Content

MODULE 1: DRUGS ACTING ON METABOLIC PROCESS, CELL WALL, AND SPECIFIC ENZYMES 15 Hrs.

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids, and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a) Drugs acting on the metabolic process:

Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone.

Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism

b)Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactum

c)Drugs acting on specific enzymes: H^+/K^+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

MODULE II: DRUGS ACTING ON GENETIC MATERIAL AND IMMUNE SYSTEM 15 Hrs.

Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.

b) DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

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g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Drugs acting on immune system: Introduction to immune system.

Immunosupressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and strucrural formula of levamisol.

MODULE III: DRUGS ACTING ON RECEPTORS AND ION CHANNELS:

15 Hrs.

Introduction, targets for drug action, receptor concept. Receptor families-structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors

Drugs acting on receptors:a)Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin.

β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.

b)Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists-. Synthesis of Acetyl choline and Succinyl choline

c)Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists- Synthesis of L-Dopa and Chlorpromazine.

d)Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.

e)Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.

f) Hormones and their receptors: Introduction to oestrogen receptors, Structural formulae of Tamoxifen

Drugs acting on ion channels: drugs acting on Ca^{2+}, Na^{+} and Cl^{-} channels and their Mode of action. synthesis of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

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5. References:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye etal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders.

6. Syllabus Focus

a) Relevance to Local, Regional, National and Global Development Needs

Local/Regional/National /Global Development Needs	Relevance
LOCAL	Optimizing existing drugs, advancement of new synthetic processes, development of new materials with enhanced properties
REGIONAL	Designing new drugs from SAR drive innovation in computational and medicinal chemistry
NATIONAL	Formulating symbiosis, understanding drug activities in the regulation of pharmacodynamic and pharmacokinetic properties, innovation in healthcare
GLOBAL	Improved energy efficiency and sustainability, development of new synthetic strategies, broad implications for industries and technologies

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b) Components on Skill Development/Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No. 1	Medicinal chemists play a crucial role in the drug discovery process through the selection and synthesis of compounds that establish structure–activity relationships and achieve efficacy and safety in preclinical testing
EMP	Module No.2	Involves the study of the effects of drugs on the genetic material.
ED	Module No. 3	Involves the study of the effects of drugs on the nervous system, with the goal of developing compounds that offer therapeutic benefit in humans with psychiatric and neurological disease.

7. Pedagogy

S. No	Student Centric Methods Adopted	Type / Description of Activity
1.	Problem Solving	Case studies
2.	Participative Learning	Presentation
3.	Experiential Learning	Field Trips

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8. Course Assessment Plan

a. Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA- 40%	EndSemesterExamination-60%
CO1	CIA-1 - Written Exam	Written Exam
CO2	CIA-2 – Assignment	
CO3	CIA-2 – Presentations	

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b) Model Question Paper - End Semester Exam

DRUG SYNTHESIS AND MECHANISM OF ACTION

MODEL QUESTION PAPER

THEORY

Course Code: P24/CHE/DSC/402 **Max Marks:60**

Credits: 3

SECTION A - INTERNAL CHOICE **3Q X 12= 36M**

Question Number	Module	Question	CO	BTL
1	Module 1	a) What is enzyme inhibition and write the different types of Enzyme inhibition b) Outline the synthesis of sulfomethoxazole and dapsone	CO 1	Level I Level II
2	Module 1	2. a) Describe Folate mechanism in bacteria. b) What are H+/K+ ATPase inhibitors? Give the synthesis of Omeprazole	CO 1	Level II Level I
3	Module 2	3. a) What are DNAintercalating agents? Give two examples b) Outline the mechanism of Action of AZT and write its synthesis	CO 2	Level I Level II
4	Module 2	4.a) How do you plan for the synthesis of Ciprofloxacin? What is its mechanism of action? b) What are Immunosupressing agents? Explain by taking one example.	CO 2	Level I Level I

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5	**Module 3**	5.a) Explain about Dopamine receptors and their classification. Write a short note on the Synthesis of Chlorpromazine b) Outline the Structural formulae of Tamoxifen?	**CO 3**	**Level I** **Level II**
6	**Module 3**	6.a) What are the different types of ion channels? Write the synthesis of tetracaine? b)Explain the Synthesis and pharmacological activity of Propranolol and Atenolol	**CO 3**	**Level I** **Level II**

SECTION B - ANSWER ANY 4 OUT OF 6 **4Q X 6M = 24 M**

(To compulsorily have Two question from each module)

7	**Module 1**	Explain about Macromolecular targets	**CO 1**	**Level II**
8	**Module 1**	Outline the synthesis of Acetozolamide	**CO 1**	**Level II**
9	**Module 2**	What are antiprotozoal drugs? Write the Synthesis of Metronidazole.	**CO2**	**Level I**
10	**Module 2**	Outline the structural formula and importance of Erythromycin and Streptomycin	**CO 2**	**Level II**
11	**Module 3**	Give the definition and examples of agonist and antagonist.	**CO 3**	**Level I**
12	**Module 3**	What are cholinergic receptors? Write their classification	**CO 3**	**Level I**

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b. Model Question Paper **End Semester Exam**

PAPER-II DRUG SYNTHESIS AND MECHANISM OF ACTION

Course Code: P24/CHE/DSC/402
Credits: 3

Max Marks:60
Max Hours:2½hrs

I. Answer the following (Essay Questions) 3x12=36 marks

1. a) What is enzyme inhibition and write the different types of Enzyme inhibition **(CO1) (Level I)**
   b) Outline the synthesis of sulfomethoxazole and dapsone **(CO1) (Level II)**

OR

2. a) Formulate Folate mechanism in bacteria. **(CO1) (Level I)**
   b) What are H+/K+ ATPase inhibitors? Give the synthesis of Omeprazole **(CO1) (Level II)**

3. a) What are DNAintercalating agents? Give two examples **(CO2) (Level 1)**

   b) Briefly discuss the mechanism of Action of AZT and write its synthesis **(CO2) (Level II)**

OR

4.a) How do you plan for the synthesis of Ciprofloxacin? What is its mechanism of action? **(CO2) (Level II)**
   b) What are Immuno supressing agents? Explain by taking one example. **(CO2) (Level I)**

5. a) Discuss about Dopamine receptors and their classification. Write a short note on the Synthesis of Chlorpromazine **(CO3) (Level I)**
   b) Outline the Structural formulae of Tamoxifen? **(CO3) (Level II)**

OR

6. a) What are the different types of ion channels? Write the synthesis of tetracaine? **(CO3) (Level IV)**

a) Explain the Synthesis and pharmacological activity of Propranolol and Atenolol **(CO3) (Level V)**

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II. Answer any four of the following(Short Answer Questions) 4x6=24 Marks

7. Write about Macromolecular targets. **(CO1) (Level I)**
8. Outline the synthesis of Acetozolamide**(CO1). (Level II)**
9. What are antiprotozoal drugs? Write the Synthesis of Metronidazole. **(CO2). (Level I)**
10. Write the structural formula and importance of Erythromycin and Streptomycin **(CO2). (Level II)**
11. Give the definition and examples of agonist and antagonist. **(CO3) (Level II)**
12. What are cholinergic receptors? Write their classification **(CO3) (Level II)**

c. Question Paper Blueprint

Modules	Hours Allotted in the Syllabus	COs Addressed	Section A (No. of Questions)	Total Marks	Section B (No. of Questions)	Total Marks
1	15	1	2	12	2	4 x 6 = 24
2	15	2	2	12	2	
3	15	3	2	12	2	

9. CO-PO Mapping

CO	PO	Cognitive Level	Classroom sessions (hrs)
1	1	Application	15
2	2	Evaluation	15
3	2	Evaluation	15

Prepared by Course Teacher [Name & Signature]	Checked &verified by HOD [Name & Signature]	Approved by the Principal
M. Bhargavi Dr. M. Bhargavi K. Susmitha Dr. K. Susmitha	D. Sumalatha Dr.D.Sumalatha	Dr. Uma Joseph

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Department of Chemistry
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Hyderabad-500 007.

SEMESTER-IV

POLYMERS AND DYES

1.Course Description

Programme: M.Sc.
Course Code: P24/CHE/DSE/402
Course: DSE-6
No. of credits: 3

Max. Hours: 45
Hours per week: 3
Max. Marks: 100

2. Course Objectives

- To understand Classification of Polymers, Types of polymerization and Natural and synthetic rubbers.
- To impart knowledge of different functional polymers and membranes.
- To understand nomenclature and classification of synthetic dyes.

3. Course Outcomes

CO1: Classify Polymers and study of Types of polymerization methods with mechanism. **(UNDERSTANDING)**

CO2: Describe different functional polymers and membranes. **(UNDERSTANDING)**

CO3: Acquire the knowledge about the different types of Dyes. **(UNDERSTANDING)**

4.Course Content

MODULE 1:ORGANIC POLYMERS – I

15 Hrs

Introduction, Classification of Polymers – according to origin, structure, intermolecular interactions. Types of polymerization – addition, condensation, radical, ionic and coplymerization with mechanism, Ziegler-Natta polymerization with mechanism. Stereochemistry of polymers, Plasticity – types of plastics. Molecular mass of polymers. Resins and plastics – Polystyrene and styrene copolymers, poly(vinyl chloride/vinyl acetate)and related polymers, acrylic polymers, polyesters, phenol-formaldehyde polymers, polyurethanes and epoxide polymers with examples. Natural and synthetic rubbers.

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MODULE 2: ORGANIC POLYMERS - II 15 Hrs

a) Functional polymers :
i) Electrically conducting polymers: Introduction, basic principles. Brief description of polyanilines, polypyrroles, polyacetylenes, polythiophenes and their applications.
ii) Photoconductive polymers: Liquid crystal polymers, smectoc, nematicamd cholesteric Structures, ion-exchange polymers – cationic, anionic exchange polymers and their uses.
iii) Smart materials: Uses in sensing device and communication networks.
iv) Biodegradable polymers: Definition, classification. Brief description polyhydroxyalkanoates, polycaprolactones, polyactic, polyvinyl alcohol and their applications.
b) Membranes: Filtration, micro, ultra, nano filtration. Separation of gases- Permeselectivity and gas permeability representative polymers. Liquid separation-dialysis, electroosmosis and reverse osmosis.
c) Fire retarding polymers and photonic polymers.
Polymers in biomedical application, artificial organs and controlled drug delivery

MODULE 3: DYES 15 Hrs

Synthetic and Natural dyes

Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromospheres and auxochromes with suitable examples, Witt's theory, Armstrong's theory, Baeyer's theory, Nietzki's theory, Waston's theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methanedyes [malachite green, rosaniline, para aniline blue, crystal violet methyl violet, hydroxytriphenyl methane dyes, Aurin, chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.

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Osmania University
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5. References

1. Organic polymer chemistry by K.J.Sanders.
2. Polymer syntheses, Vol.I by S.R.Sandler and W.Karo
3. The elements of Polymer Science and Engineering by A.Rudin
4. Principles of Polymer Chemistry by A.Ravve
5. Polymer Science by V.R.Gowariker , N.V.Viswanathan and J.Sreedhar
6. Polymer Chemistry by C.E.Carraher , Jr.
7. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar , S. Chand
8. Polymer Chemistry, B. Vollmert
9. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
10. Organic Chemistry , Vol.1,2 by I.L.Finar
11. Color and constitution of organic molecules by J.Griffiths
12. Functional Dyes, Elsevier BV 2006S H.KIM
13. Colorants for non-textile Applications, Elsevier BV 2000 …H S Freeman and A T Peters
14. Industrial Dyes-Chemistry, Properties, Applications. WILEY-VCH Verlag, 2003
15. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
16. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers.

Prepared by Course Teacher [Name & Signature]	Checked &verified by HOD [Name & Signature]	Approved by the Principal
Dr. Sabiha Fatima	Dr.D.Sumalatha	Dr. Uma Joseph

Head
Department of Chemistry
UCS, Osmania University
Hyderabad-500 007.

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DEPARTMENT OF CHEMISTRY

PROJECT

1.Course Description

Programme: M.Sc. Organic Chemistry
Course Code: P24/CHE/PRJ/401
Course: PRJ
No. of credits: 5

Max. Hours:
Hours per week: 5
Max. Marks: 150

PROJECT

COURSE OUTCOMES

CO1: Assimilate the required skills through theoretical & practical knowledge during the project work.

CO2: Gain the required ability to start up own industry and comprehend the ability to draft and communicate the practical work.

- The project will be performed at the established industry (or) in the department under the supervision of the faculty or research institutes.
- It may involve experimental and/or theoretical work as well as critical review of the literature.
- Each of the students has to carry out original research in a topic in accordance with the work chosen under the guidance and supervision of a teacher in the concerned department of the college.

SEMESTER-IV PRACTICALS

CHEMISTRY LAB: DSC- 11

LAB: SYNTHESIS OF DRUGS

Program: M.Sc.
Course: DSC-11
Semester: 4

Subject Code P20/CHE/DSC/401/P
No. of Hrs. allotted: 4 Hrs / week
No. of Credits :2

COURSE OUTCOMES

This course will help the students to

CO1. Describe organic chemical reactions and explain their associated reaction mechanisms and apply this to drug molecules.
CO2: Importance of synthesis of drugs in day today life.

Synthesis of the following Drugs :

1. Paracetamol
2. Phenytoin
3. Benzocain
4. Chloritone
5. 4-Aminobenzene
6. Sulfonamide
7. Antipyrine
8. Phenothiazine
9. 2,4,5 tri phenyl imidazole
10. 4- Chloro benzhydryl piperazine

Reference books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel

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SYNTHESIS OF DRUGS

PRACTICAL MODEL QUESTION PAPER

Course Code: P24/CHE/DSC/402/P
Credits: 2

Max Time:3hrs
Max marks :50 marks

Answer all questions.

1. Write the principle involved in the preparation of the given Drug molecule. **10M (CO1& CO2)**

2. Synthesize the given Drug molecule and report its melting point. **25M (CO1)**

3. Record + Attendance **5M**

4. Viva 10M **(CO1 & CO2)**

Prepared by	Checked & verified by	Approved by
Name and Signature of the teaching faculty	Name and Signature of HoD	Name and Signature of Principal
Dr. K.Susmitha Dr.M. Bhargavi	D. Sumalatha Dr. D. Sumalatha	Dr. Uma Joseph

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Department of Chemistry
UCS, Osmania University
Hyderabad-500 007.